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SIMULATION OF CO_2 RELEASE AT 800 KM ALTITUDE

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13. ABSTRACT (*Maximum 200 words*)

The SOCRATES contamination-interaction code has been used to simulate the reactions of $O + CO_2 \rightarrow CO_2(\upsilon) + O$, $O + CO_2 \rightarrow CO(\upsilon) + O_2$, and $CO_2 + H \rightarrow CO + OH(\upsilon)$ at an altitude of 800 km in both ram and wake directions of the spacecraft. These simulations show that the radiation from these reactions can be measurable for the parameters which have been used in these calculations. The investigation carries out the simulations as much as 30 km from the spacecraft. The radiative intensity of $CO(\upsilon)$ and $OH(\upsilon)$ show the highest and lowest, respectively.

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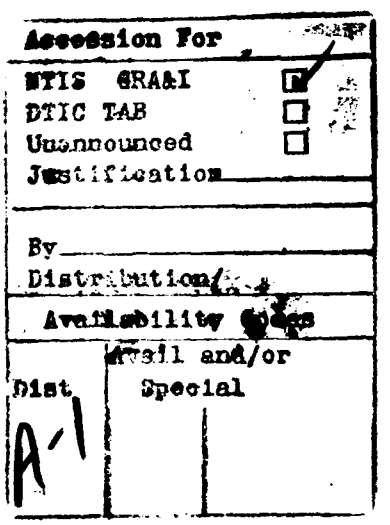
TABLE OF CONTENTS



LIST OF FIGURES

LIST OF TABLES

1. INTRODUCTION

The present work is based on simulation of CO_2 released at an altitude of 800 km in both the ram and wake directions of the spacecraft using the SOCRATES (Spacecraft/Orbiter Contamination Representation Accounting for Transiently Emitted Species) code. SOCRATES is a Monte Carlo code which calculates scattering, collisional excitations, and reactive collisions [*Elgin, et al.*, 1990]. The code will be discussed in more detail later. The primary purpose of the simulation is to study the collisional excitation of CO_2 with atmospheric oxygen and hydrogen atoms. The reactions of CO_2 with oxygen can produce the vibrational excitation of CO_2 and CO. Similarly, the CO_2 reaction with hydrogen atoms produce vibrationally-excited OH. This parametric study is a continuation of earlier work on the subject [*Setayesh*, 1991]. The current investigation carries out the simulations in two directions to a distance of as much as 30 km from the point of origin. The reactions of CO_2 with atomic oxygen and hydrogen are:

$$O_{fast} + CO_2 \rightarrow CO\ (v) + O_2 \qquad (1)$$

$$H_{fast} + CO_2 \rightarrow OH\ (v) + CO \qquad (2)$$

$$O_{fast} + CO_2 \rightarrow CO_2\ (v) + O_{slow} \qquad (3)$$

Reaction (4) represents the collisional transfer of kinetic energy to vibrational energy. Reactions (5) and (6) are reactive collisions which do not proceed at room temperature due to large activation energies [*Elgin, et al.*, 1990].

2. DESCRIPTION OF THE MODEL CONFIGURATION

The model configuration is based on a proposed gas release experiment on the ARGOS satellite. The satellite is expected to be in a circular orbit at an altitude of approximately 800 km with an orbital velocity of 7.4 km/s. The CO_2 release experiment will be one of many experiments to be conducted onboard the satellite [*Lai, et al.*, 1992]. A nozzle with a small diameter is assumed to be the source of the CO_2 gas released into space from a space platform. The diameter of the nozzle and mass flow rate of the CO_2 remain constant. Two conditions for the release will be considered here: one in the ram direction, and the other in the wake direction. It is also assumed that the gas release will last approximately 1.0 second (from a fraction of a second to several seconds has been proposed in the actual experiment). The temperature of the CO_2 gas at the time of the release is assumed to be about 50° C. The solution domain in the steady state (for both reactions) is taken to be a cubic space of 28,800 km^3 in volume (32 by 30 by 30 km^3) consisting of 8400 unevenly spaced cells. In each cell, there are 3 to 20 molecules (depending upon the density of species and cell location) for each species.

3. DESCRIPTION OF THE SOCRATES CODE

The SOCRATES contamination-interaction code has been developed to model contamination on spacecraft and to study the neighboring flow field around the shuttle [*Elgin and Sundberg*, 1988]. In the SOCRATES code, the direct simulation Monte Carlo technique has been revised and extended significantly to account for the energy dependent collision cross sections [*Bird*, 1981] and a statistical collision model for internal energy effects [*Borgnakke and Larsen*, 1975] which have been described by *Elgin and Sundberg* [1988] and *Elgin, et al.*, [1990]. In the code, the collision cross section is defined by the variable hard sphere model (VHS) which is a function of the relative velocity between two molecules. The collision cross section can be stated as

$$\sigma = \sigma_{ref} \left(\frac{v_r}{v_{ref}}\right)^{-2\omega} \quad (4)$$

where σ_{ref} and v_{ref} are the reference collision cross section and velocity, respectively [*Elgin, et al.*, 1990]. ω is a constant parameter which has a value of 0.25 for this investigation.

Reactive collisions between molecules and/or atoms (which are relevant to the present work) can be simulated directly by SOCRATES. The reaction cross section is a function of the relative collision energy as defined by Equation (4). The Monte Carlo program, in the event of collision, simulates the reaction with a probability which is related to the ratio of the reactive cross section to collision cross section at the relative velocity for the collision [*Elgin and Sundberg*, 1988].

The present work employs the option of using the Arrhenius rate constant in the code to calculate the rate of reactive collisions. The rate constant has the form of

$$k_r = A\ T^n\ e^{-\frac{E_a}{R_0 T}} \quad (5)$$

where A and n are constant parameters, R_0 and T are gas constant and temperature, respectively, and E_a is the activation energy. In the case of the collision between two reactants, the reaction cross section is calculated, and the reaction is counted with a weighing factor W_r. The weighing factor is given by

$$W_r = W_c \frac{v_r\ \sigma^*}{v_r\ \sigma} \quad (6)$$

where σ^*, σ, and W_c are the reactive cross section, collision cross section, and collision weighing factor, respectively. Further discussion of the reactive collisions can be found in the report by *Elgin and Sundberg* [1988].

4. DISCUSSION OF RESULTS

The simulation for the reaction of CO_2 with O and H for the altitude of 800 km are presented in panels of tables and plots for two cases of ram and wake directions. Tables 1-3 represent the parameters used for the simulation. Figures 1-3 and 5-7 show panels of contour plots of radiation intensity and reaction rates for CO_2, CO, and OH, respectively, in the ram and wake directions. Figures 4 and 8 show the combination of cases presented in Figures 1-3 and 5-7, respectively. Figure 9 shows the gray plot for CO_2 density distribution in the ram and wake directions. The asterisks in the figures and the text denote vibrational excitations.

Table 1 shows the reference collision cross-section σ_{ref}, reference relative collision velocity v_{ref}, number of internal degrees of freedom v_i, and heat formation for the species.

TABLE 1. Molecular Parameters Used in the Calculations

Species	σ_{ref} cm^2	v_{ref} cm/s	v_i	Heat of Formation kcal/mole
CO_2	4.33×10^{-15}	1.71×10^5	3.58	-94.10
O	1.75×10^{-15}	2.49×10^5	0.00	59.60
H	1.03×10^{-15}	1.09×10^6	0.00	52.0
CO_2(4.3)	4.33×10^{-15}	1.71×10^5	3.58	-87.39
CO(4.7)	3.46×10^{-15}	2.09×10^5	2.00	-20.29
O_2	3.17×10^{-15}	1.98×10^5	3.60	0.0
OH(2.7)	1.77×10^{-15}	8.00×10^5	2.00	9.4

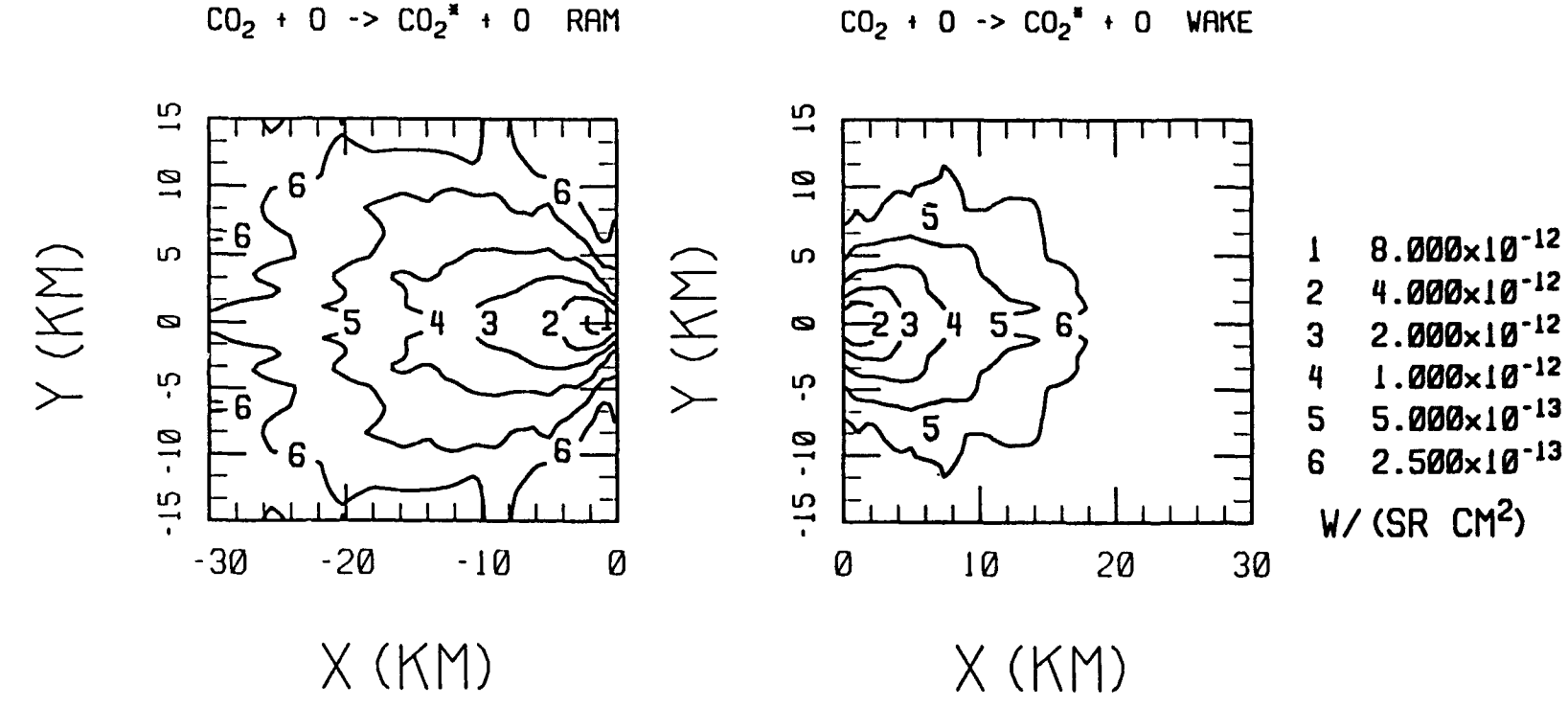


Figure 1. Contour plots showing the CO_2 vibrational excitations at 4.3 μm.

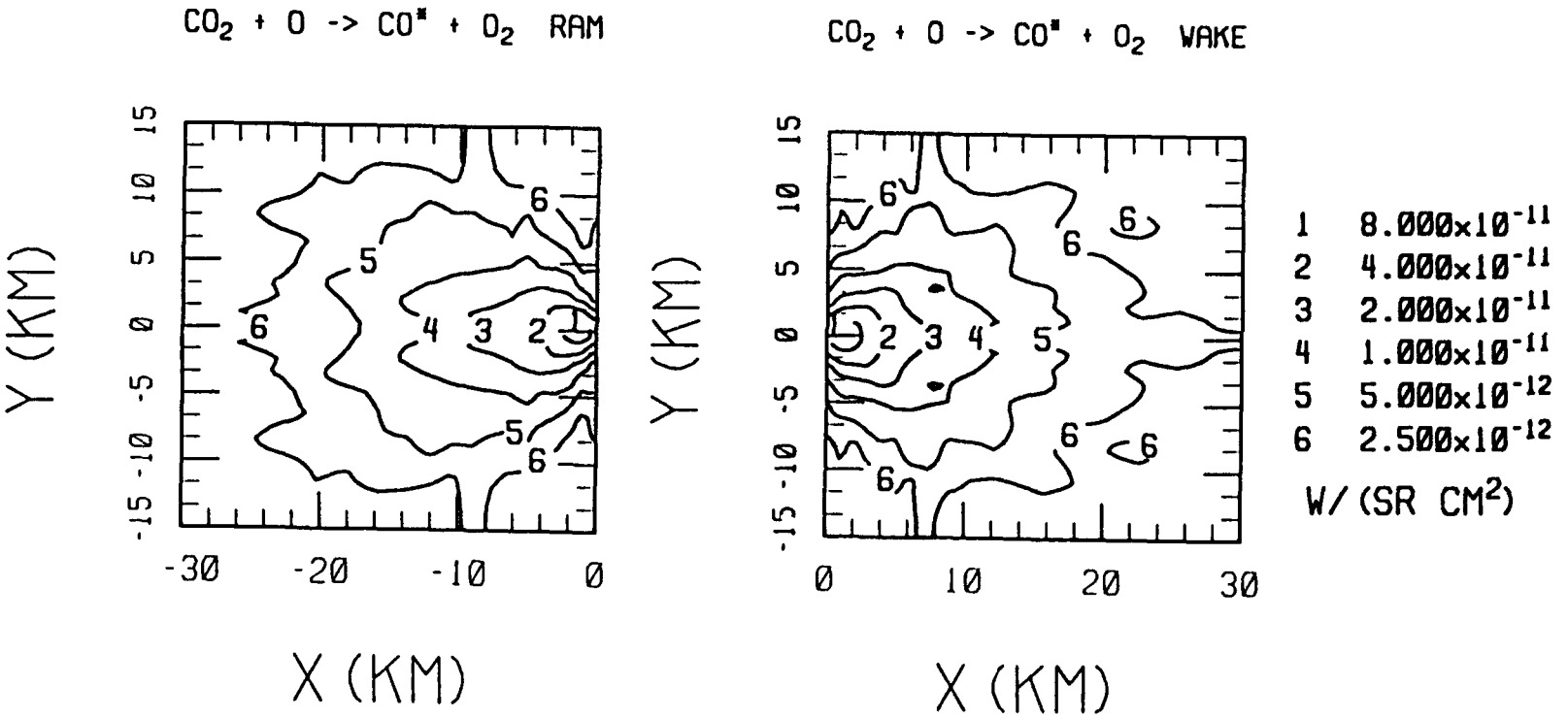


Figure 2. Contour plots showing the CO vibrational excitations at 4.7 μm.

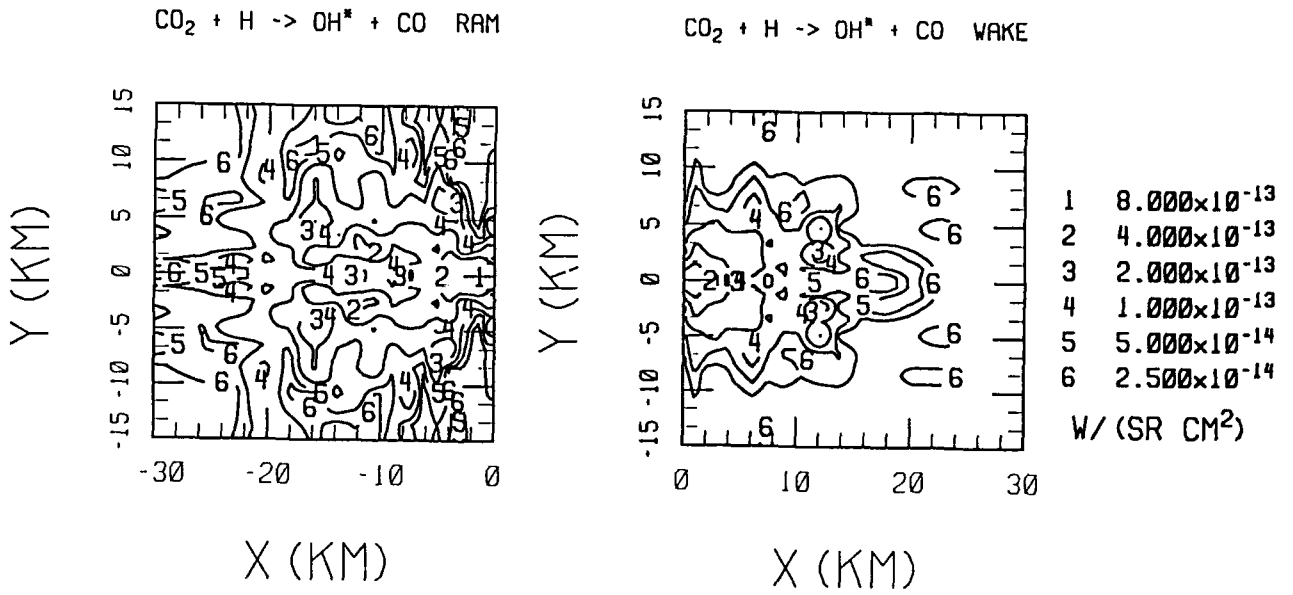


Figure 3. Contour plots showing the OH vibrational excitations at 2.7 μm.

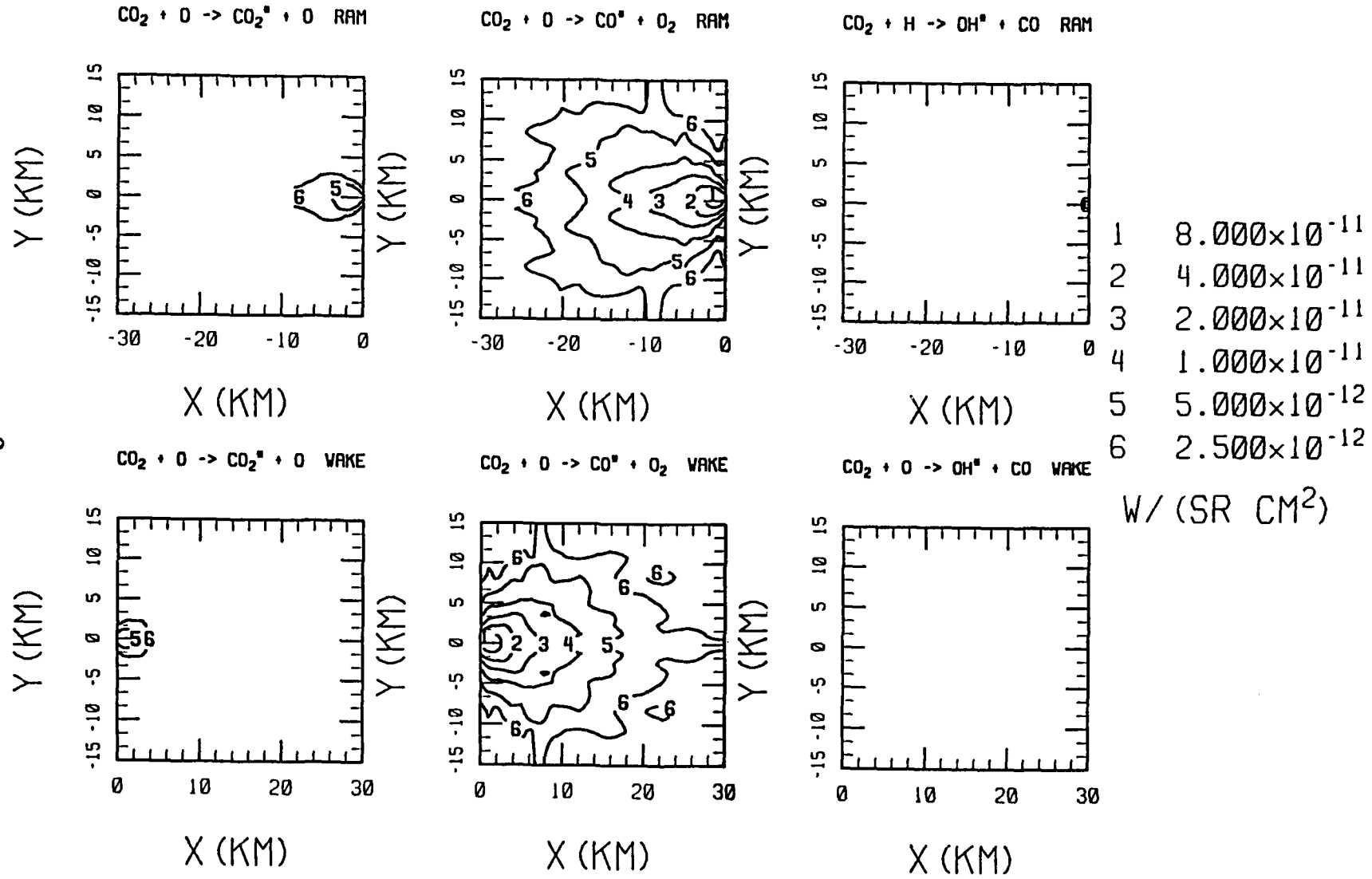


Figure 4. Contour plots showing the CO_2, CO, and OH vibrational excitations for the same scale.

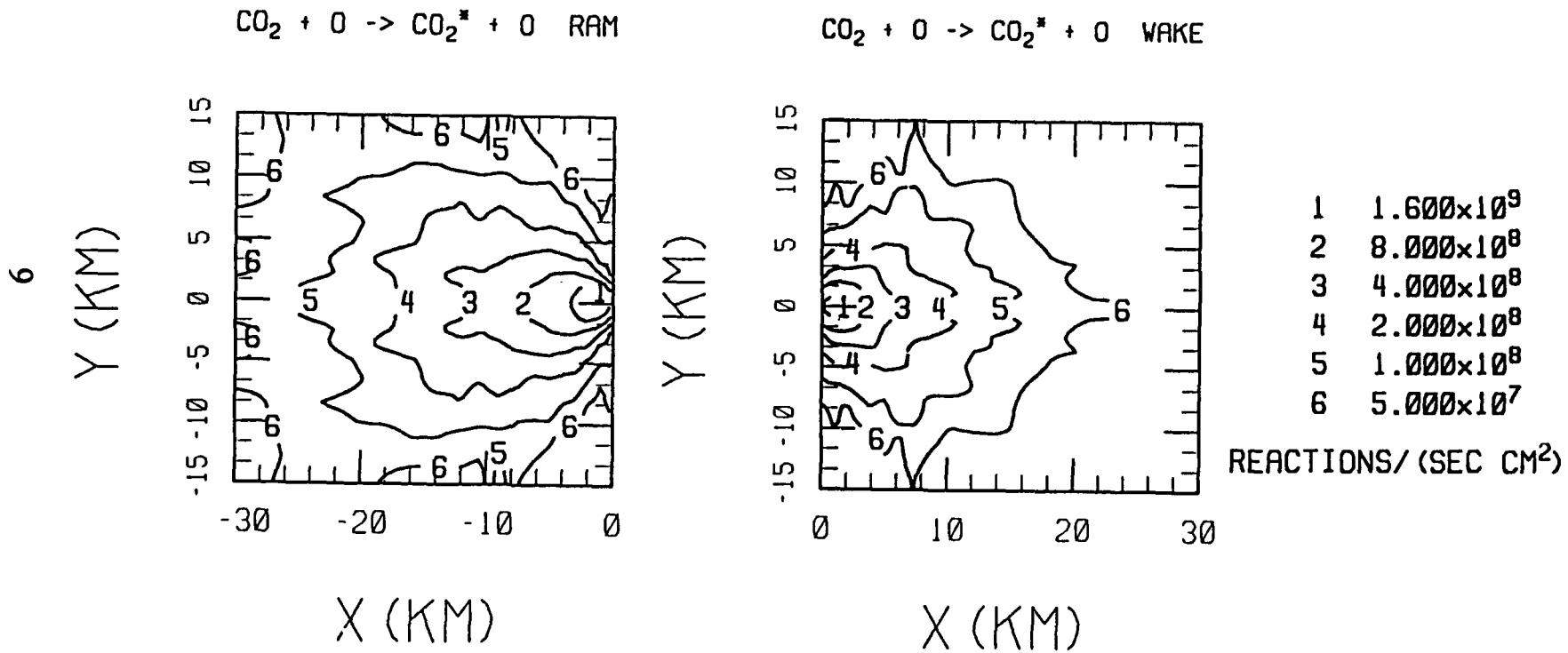


Figure 5. Contour plots showing the CO_2 reaction rates.

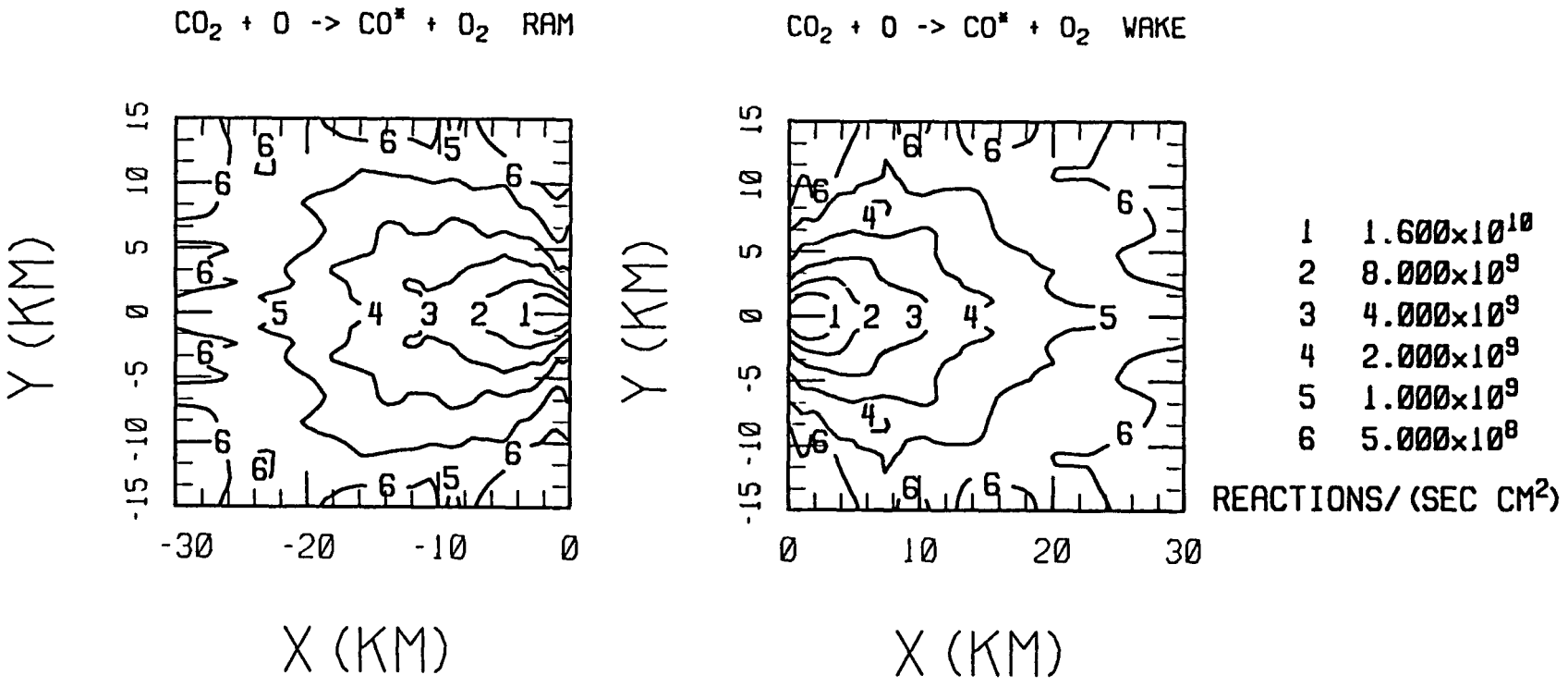


Figure 6. Contour plots showing the CO reaction rates.

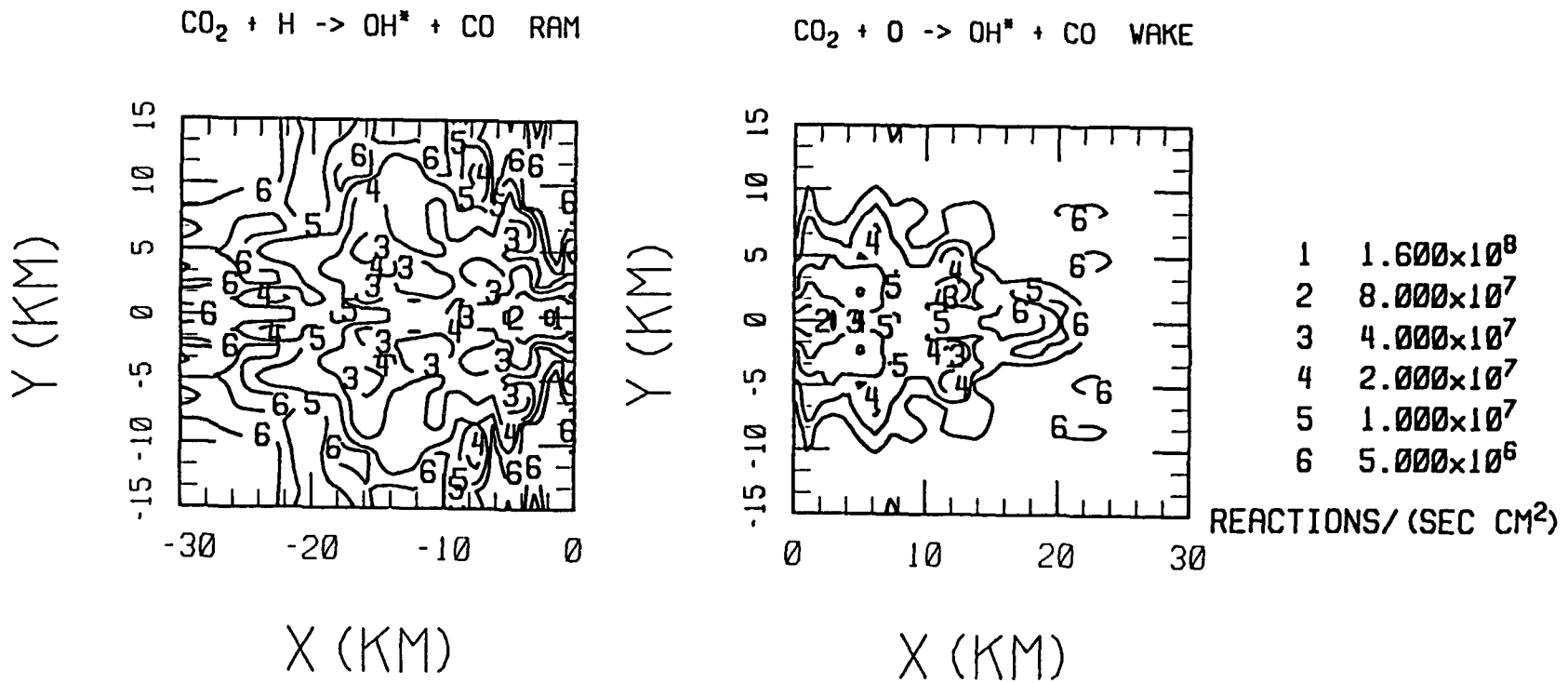


Figure 7. Contour plots showing the OH reaction rates.

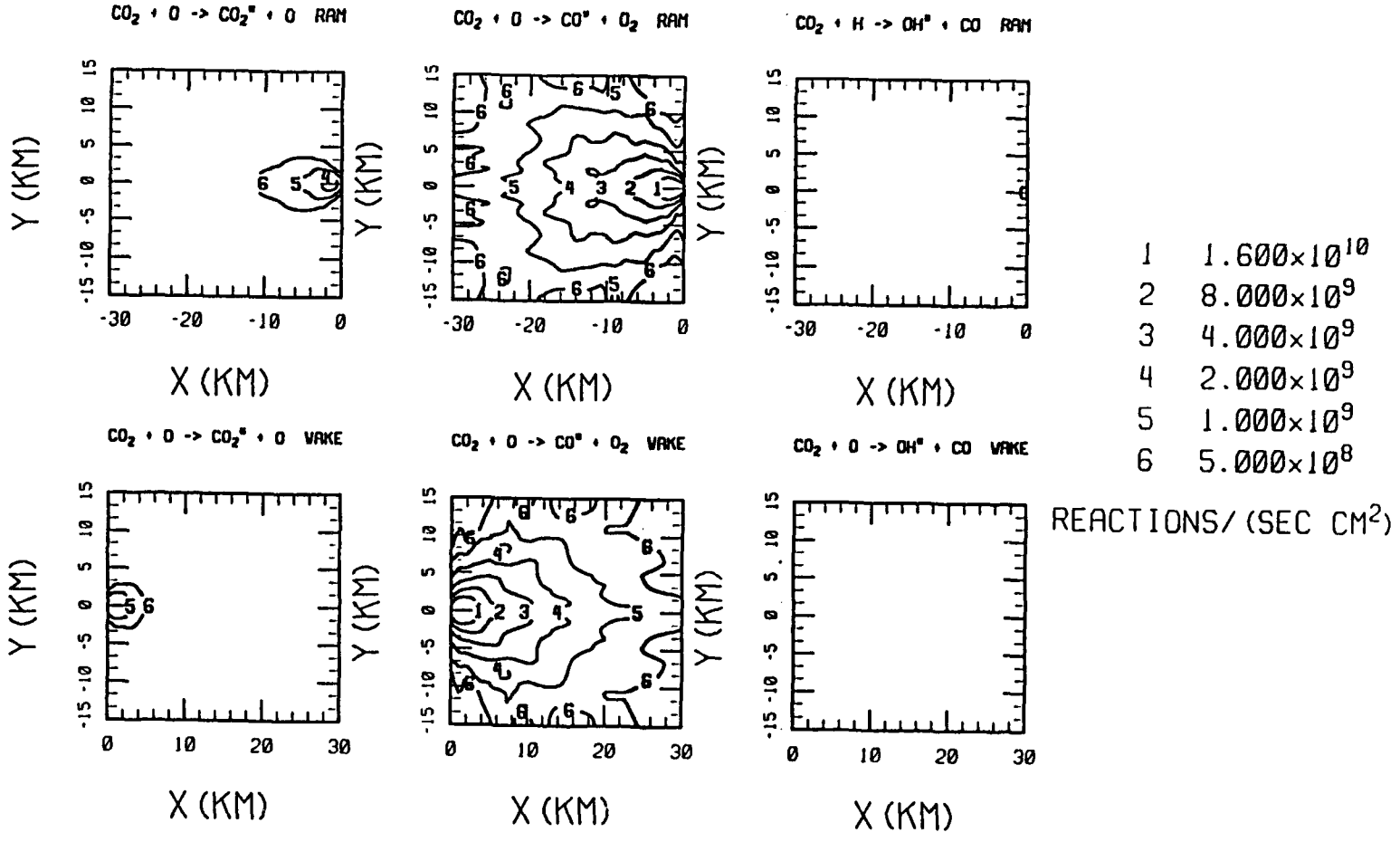


Figure 8. Contour plots showing the CO_2, CO, and OH reaction rates for the same scale.

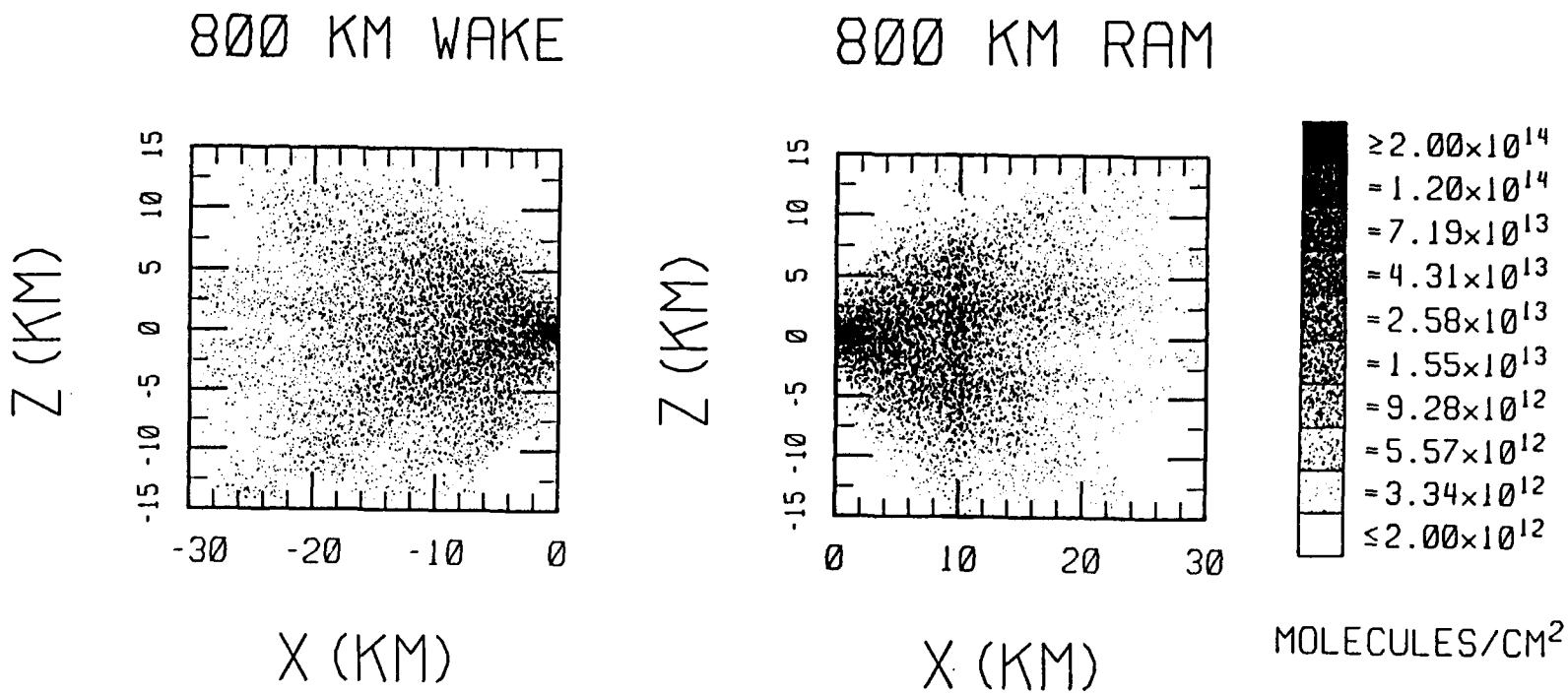


Figure 9. Gray scale plots showing the intensity of CO_2 at the time of release.

Table 2 shows the values used in Arrhenius Rate Coefficients for the different reactions, where A, n, and k are constant parameters, T is temperature, and E_a is the activation energy.

TABLE 2. Rate Coefficient Used in SOCRATES, $k = A\ T^n \exp(-E_a/kT)$

Reaction	A	n	E_a (kcal/mole)
$O_{fast} + CO_2 \rightarrow CO_2(v) + O_{slow}$	3.9×10^{-20}	1.8	6.71
$O_{fast} + CO_2 \rightarrow CO(v) + O_2$	5.6×10^{-11}	0.0	14.21
$H_{fast} + CO_2 \rightarrow CO + OH(v)$	2.5×10^{-10}	0.0	26.43

Table 3 lists the other parameters that have been used in SOCRATES to simulate CO_2 released from a 5 mm diameter nozzle with a mass flow rate of 144 g/s.

TABLE 3. Parameters Used in the Simulations

Atmospheric Temperature	1002.3°K
Atmospheric Number density	2.047×10^6 cm^{-3}
Altitude	800 km
Mass Flow	144.0 g/s
Exit Plane Area	2.5×10^{-1} cm^2
Ratio of Specific Heat	1.30
Exit Mach Number	1.40
Exit Nozzle Half Angle	22.5 degrees
Exit Plane Density	1.789×10^{-2} g/cm^3
Exit Plane Number Density	2.448×10^{20} molecules/cm^3
Exit Plane Velocity	410.0 m/s
Exit Plane Speed of Sound	2.929×10^4 cm/s
Exit Plane Temperature	350.0°K
Exit Plane Pressure	1.18×10^7 dyne/cm^2
Stagnation Temperature	451.9°K
Stagnation Pressure	3.607×10^7 dyne/cm^2
Thrust	18.5 lb
Velocity of Spacecraft	7.4 km/s

Figure 1 shows the emission at 4.3 μm from vibrational excitation of CO_2 produced by collisional energy between O atoms and released CO_2 molecules. Figures 2 and 3 show the emission from the reactive collisions between CO_2 and O and H atoms, respectively. Figure 2, the CO^* emission at 4.7 μm, shows one order of magnitude higher rate of emission with respect to CO_2^* in Figure 1. This is because the radiative lifetime of CO^* is of the order of μs compared with CO_2^* whose radiative lifetime is of the order of ms. The emission rate of OH^* at 2.7 μm in Figure 3, is smaller than the rates of CO^* and CO_2^* (Figures 1 and 2). The rate coefficient given in Table 2 was used to calculate the contours in Figures 1 and 2. The contour plots shown in the figures are in the two directions of ram and wake, where in the ram direction, the flow has a relatively larger initial upstream velocity component, and this contributes to higher-energy collisions; hence, higher levels of emission are produced. Figure 4 is a combination of the plots of Figures 1, 2, and 3 with the same scale for the energy levels. As it is seen in this figure, the emission rate (watts per steradian per cm^2), of CO^* is much higher than that of CO_2^* and OH^* .

Figures 5, 6, and 7 show the reaction rate per sec per cm^2 for reactions 4, 5 and 6. As expected, the intensity of the reactions are similar to those of the emissions in Figures 1, 2, and 3, respectively. Figure 8 represents the combination of the reaction rates in Figures 5, 6, and 7, which is plotted with the same scale. As it is seen, the intensity in reaction 5 for CO^* is much higher than for CO_2^* and OH^* in reactions 4 and 6, respectively. Figure 9 represents the intensity of CO_2 molecule distributions per cm^2 at the time of release, in the two directions of ram and wake.

5. SUMMARY AND CONCLUSIONS

A bundle of CO_2 gas was assumed to be released from a nozzle with a small diameter at high altitude. The diameter of the nozzle and mass flow rate are assumed to be 5 mm and 144 g/s, respectively, in this parametric investigation. The reactions $O + CO_2 \rightarrow CO_2(v) + O$, $O + CO_2 \rightarrow CO(v) + O_2$, and $CO_2 + H \rightarrow CO + OH(v)$ were simulated for the above cases from an altitude of 800 km, using the SOCRATES contamination-interaction code. The results were presented in forms of graphs, contour, and gray scale plots for these simulations. These simulations show that the radiation from these reactions should be measurable for the parameters which have been used in these calculations.

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